cis-Phenanthrene, 9,10-dihydro-9-methyl-9,10-diol, diacetate

Inchi: InChI=1S/C19H18O4/c1-12(20)22-18-16-10-5-4-8-14(16)15-9-6-7-11-17(15)19(18,3)23-1

InchiKey: JRAOUDMKMKUKMH-RBUKOAKNSA-N

Formula: C19H18O4

SMILES: CC(=O)OC1c2ccccc2-c2ccccc2C1(C)OC(C)=O

Mol. weight [g/mol]: 310.34

Physical Properties

Property code	Value	Unit	Source
gf	-93.53	kJ/mol	Joback Method
hf	-401.11	kJ/mol	Joback Method
hfus	32.85	kJ/mol	Joback Method
hvap	80.36	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	3.750		Crippen Method
mcvol	235.070	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	2200.00		NIST Webbook
tb	848.06	K	Joback Method
tc	1087.02	K	Joback Method
tf	567.21	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.94	J/mol×K	848.06	Joback Method
cpg	719.19	J/mol×K	887.89	Joback Method
cpg	735.04	J/mol×K	927.71	Joback Method
cpg	750.68	J/mol×K	967.54	Joback Method
cpg	766.30	J/mol×K	1007.36	Joback Method
cpg	782.09	J/mol×K	1047.19	Joback Method
cpg	798.21	J/mol×K	1087.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R109589&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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